

Superconductor-Ferromagnet Bi-Layers: a Comparison of s -Wave and d -Wave Order Parameters

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Abstract. We study superconductor-ferromagnet bi-layers, not only for s -wave but also for d -wave superconductors. We observe oscillations of the critical temperature when varying the thickness of the ferromagnetic layer for both s -wave and d -wave superconductors. However, for a rotated d -wave order parameter the critical temperature differs considerably from that for the unrotated case. In addition we calculate the density of states for different thicknesses of the ferromagnetic layer; the results reflect the oscillatory behaviour of the superconducting correlations.

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1. Introduction

The interplay of superconductivity and ferromagnetism has been studied for many years [1, 2]. Nowadays the focus is on hybrid-structures of superconductors and various ferromagnetic materials. For bi-layers consisting of a superconductor and a ferromagnetic metal an oscillation of the critical temperature has been found – experimentally [3, 4, 5] as well as theoretically [6, 7] – when increasing the thickness of the ferromagnetic layer. Similar observations have been made for superconductor-ferromagnet multi-layers [8, 6]. For two superconductors which are coupled via a thin layer of a ferromagnetic metal an oscillation of the critical current when varying the layer thickness has also been reported [9, 10]; depending on the layer thickness such systems can be π -junctions. Recently a layer of a ferromagnetic metal attached to a bulk superconductor has been considered, resulting in the density of states showing oscillations [11, 12, 13, 14], too. The origin of these effects is a state in the ferromagnetic metal which is similar to that proposed for a ferromagnetic superconductor by Larkin and Ovchinnikov [2] and Fulde and Ferrell [1]: in the presence of a spin exchange field the superconducting order parameter is spatially oscillating. A LOFF-like state can be present in a ferromagnet where superconducting correlations enter via the proximity effect [7].

Up to now only s -wave superconductors have been studied. In view of possible applications, it is also important to consider an order parameter with d -wave symmetry, which presumably is realized in the cuprates; there the crystallographic orientation fixes the direction of the d -wave lobes. For a related experimental investigation see [15].

In this work we extend the theory to d -wave superconductors, where we have to account for the anisotropy of the order parameter. This means that in the quasi-classical framework, which we use, the Usadel equation is no longer applicable, and we have to use the Eilenberger equation instead. It should be mentioned that the Eilenberger equation is also needed for the description of s -wave superconductors in the clean limit, which was pointed out for the current problem in [16].

In the following we study a bi-layer of a superconductor and a ferromagnetic metal as presented in figure 1. As the structures we are interested in are three-dimensional our mean field approach is of sufficient accuracy. We consider the behaviour of the critical temperature and of the density of states. In particular we compare the results for different order parameter symmetries, namely of the s -wave and d -wave type. First we briefly introduce the fundamental quasi-classical equations. Afterwards we present the results, and we finish with a short conclusion.

2. Method

To study superconductors in the vicinity of boundaries we apply the theory of quasi-classical Green's functions in thermal equilibrium [17, 18]. The Green's functions are determined from the Eilenberger equation

$$\begin{aligned} & [\hat{\tau}_3 E + I(\mathbf{r})\hat{\sigma}_3 + i\hat{\Delta}(\mathbf{p}_F, \mathbf{r}) - \hat{\Sigma}(\mathbf{r}), \hat{g}(E, \mathbf{p}_F; \mathbf{r})] + \\ & + i\mathbf{v}_F \cdot \partial_{\mathbf{r}} \hat{g}(E, \mathbf{p}_F; \mathbf{r}) = 0. \end{aligned} \quad (1)$$

and must fulfil the normalisation condition

$$[\hat{g}(E, \mathbf{p}_F; \mathbf{r})]^2 = \hat{1}. \quad (2)$$

Here $\hat{\tau}_i$ is the direct product of the i^{th} Pauli-matrix in Nambu space and the identity in spin space; vice versa $\hat{\sigma}_i$ is the direct product of the i^{th} Pauli-matrix in spin space and the identity in Nambu space. Consequently the Green's function, \hat{g} , has a 4×4 matrix structure. For our purpose it is sufficient to choose the orientation of the internal spin-exchange field of the ferromagnetic metal in z -direction, $\mathbf{I}(\mathbf{r}) = I(\mathbf{r})\mathbf{e}_z$, which leads to the term $I(\mathbf{r})\hat{\sigma}_3$ in the Eilenberger equation.

The superconducting order parameter, which we assume to be spin-singlet, reads

$$\hat{\Delta}(\mathbf{p}_F, \mathbf{r}) = \begin{pmatrix} 0 & i\hat{\sigma}_2 \Delta(\mathbf{p}_F, \mathbf{r}) \\ -i\hat{\sigma}_2 \Delta^*(\mathbf{p}_F, \mathbf{r}) & 0 \end{pmatrix} \quad (3)$$

with

$$\Delta(\mathbf{p}_F, \mathbf{r}) = \eta(\mathbf{p}_F)\Delta(\mathbf{r}). \quad (4)$$

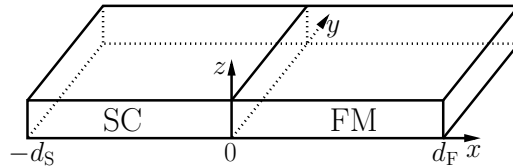


Figure 1. A bi-layer consisting of a superconductor of thickness d_S and a ferromagnetic metal of thickness d_F . The interface between both materials (at $x = 0$) is assumed to be completely transparent, and the sample is translationally invariant in y - and z -direction.

The symmetry of the order parameter is determined by the basis function, $\eta(\mathbf{p}_F)$:

$$\eta(\mathbf{p}_F) = \begin{cases} 1 & s\text{-wave}(\eta_s) \\ (p_{Fx}^2 - p_{Fy}^2)/p_F^2 & \text{unrotated } d\text{-wave } (\eta_d) \\ p_{Fx}p_{Fy}/p_F^2 & 45^\circ\text{-rotated } d\text{-wave } (\eta'_d) \end{cases} . \quad (5)$$

The order parameter must be determined self-consistently via

$$\hat{\Delta}(\mathbf{r}) = -\pi V \mathcal{N}_0 T \sum_{|E_n| < E_c} \frac{\hat{\sigma}_2}{2} \text{Tr}_\sigma \left[\hat{\sigma}_2 \langle \eta(\mathbf{p}'_F) \hat{g}(E, \mathbf{p}_F; \mathbf{r}) \rangle_{\mathbf{p}_F} \right] , \quad (6)$$

where $\langle \dots \rangle_{\mathbf{p}'_F}$ denotes an average over the Fermi surface, which is assumed to be spherical in the s -wave case and cylindrical in the d -wave case (this is justified for the layered cuprate superconductors). The cut-off energy is E_c , the attractive interaction is $V < 0$, and the normal density of states per spin at the Fermi energy is denoted by \mathcal{N}_0 . Impurity scattering is treated in Born approximation which leads to the following self-energy:

$$\hat{\Sigma}(E, \mathbf{r}) = \frac{-i}{2\tau} \langle \hat{g}(E, \mathbf{p}_F; \mathbf{r}) \rangle_{\mathbf{p}_F} \quad (7)$$

with the scattering time τ .

It is important to note that in principle the quasi-classical theory is only valid if all energy scales are small compared to the Fermi energy, E_F ; for most superconductors this is the case as $T_c \ll E_F$. However, for many ferromagnetic materials the exchange energy is of the same order of magnitude as E_F . Strictly speaking this theory can therefore only be applied for rather weak ferromagnets. Strong ferromagnets have been treated in some special cases: superconductors in proximity to half-metals (where only one spin-channel is metallic) [19] or in contact to strong ferromagnetic insulators [20, 21] have been examined by extensions of the quasi-classical theory.

3. Results

First we investigate the oscillations of the pairing function in a quite simple system which we can treat analytically: we consider a ferromagnetic layer of thickness d_F attached to a bulk superconductor ($d_S \rightarrow \infty$, see figure 1) without disorder; for simplicity we consider the case of a spherical Fermi surface in both materials, and an identical Fermi velocity, v_F . Furthermore we assume a completely transparent interface at $x = 0$, a specular surface at $x = d_F$, and a spatially constant order parameter in the superconductor, $\Delta(\mathbf{p}_F, \mathbf{r}) = \Delta(\mathbf{p}_F)$. Then the normal part of the Green's function in the ferromagnetic metal reads

$$g_{\uparrow\uparrow/\downarrow\downarrow}(E, \mathbf{p}_F) = \frac{1 - e^{i\vartheta_{\uparrow/\downarrow}(E, \mathbf{p}_F)} \alpha(E, \mathbf{p}_F) \beta(E, \mathbf{p}'_F)}{1 + e^{i\vartheta_{\uparrow/\downarrow}(E, \mathbf{p}_F)} \alpha(E, \mathbf{p}_F) \beta(E, \mathbf{p}'_F)} \quad (8)$$

with

$$\alpha(E, \mathbf{p}_F) = \frac{E - \sqrt{E^2 - |\Delta(\mathbf{p}_F)|^2}}{\Delta^*(\mathbf{p}_F)}, \quad (9)$$

$$\beta(E, \mathbf{p}_F) = -\frac{E - \sqrt{E^2 - |\Delta(\mathbf{p}_F)|^2}}{\Delta(\mathbf{p}_F)}, \quad (10)$$

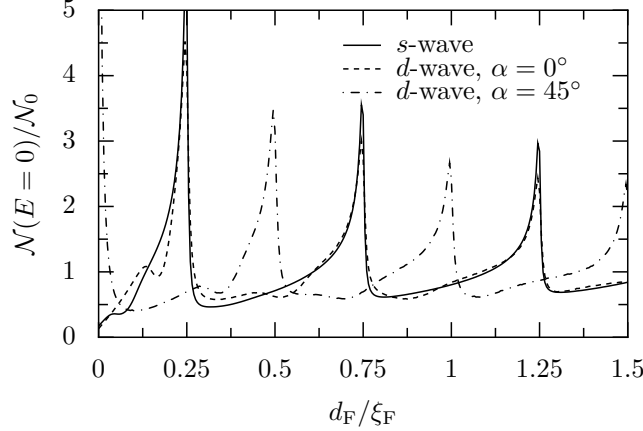


Figure 2. The density of states at $E = 0$ is shown as a function of the ferromagnetic layer thickness with $\xi_F = \pi v_F/I$. The s -wave and the unrotated d -wave case are almost identical with maxima at $d_F = (1/2 + k)\xi_F/2$, where k is an integer; for a rotated d -wave order parameter the maxima are shifted to $d_F = k\xi_F/2$. For the plot we added a finite imaginary part to the energy ($E \rightarrow E + i0.01T_c$).

and

$$\vartheta_{\uparrow/\downarrow}(E, \mathbf{p}_F) = \frac{2(E \mp I)\lambda(\mathbf{p}_F)}{v_F}; \quad (11)$$

$\lambda(\mathbf{p}_F) = 2d_F p_F / p_F^{\parallel}$ (p_F^{\parallel} : Fermi momentum parallel to the y - z -plane) is the length of the classical trajectory in the ferromagnetic layer. Note that \mathbf{p}_F' is uniquely determined by \mathbf{p}_F for a specular surface since the parallel momentum is conserved, $p_F^{\parallel} = p_F'^{\parallel}$.

The angle-resolved density of states in the ferromagnetic layer can be expressed in terms of the normal part of the Green's function,

$$\mathcal{N}(E, \mathbf{p}_F) = \frac{1}{2} \mathcal{N}_0 \text{Re} [g_{\uparrow\uparrow}(E, \mathbf{p}_F) + g_{\downarrow\downarrow}(E, \mathbf{p}_F)]. \quad (12)$$

We now consider the angle-averaged density of states at $E = 0$ as a function of d_F , which is normalised by the ferromagnetic length, $\xi_F = \pi v_F/I$. In figure 2 we present the results for the s -wave case ($\Delta(\mathbf{p}_F) = 1.76T_{c0}$) as well as for the unrotated ($\Delta(\mathbf{p}_F) = 2.14T_{c0}\eta_d(\mathbf{p}_F)$) and for the 45° -rotated d -wave cases ($\Delta(\mathbf{p}_F) = 2.14T_{c0}\eta_d'(\mathbf{p}_F)$); we choose an exchange field of $I = 10T_{c,0}$.

The zero-energy density of states for an s -wave and an unrotated d -wave order parameter behaves quite similar up to minor deviations: we find maxima at $d_F = (1/2 + k)\xi_F/2$, $k \in \mathbf{N}_0$. At these values of d_F Andreev bound states with a large spectral weight exist in the gap region; i.e. in the gap region the density of states is enhanced compared to the normal state value. For a 45° -rotated d -wave order parameter we find maxima at $d_F = n\xi_F/2$. The reason for this shift is that the quasi-particles acquire an additional phase due to the scattering at the surface which changes the sign of the order parameter. In particular for $d_F = 0$ the commonly known zero-energy bound states occur at surfaces [22].

The density of states has been studied before [12, 13, 23] including surface roughness and a finite transparency of the superconductor-ferromagnet interface. The

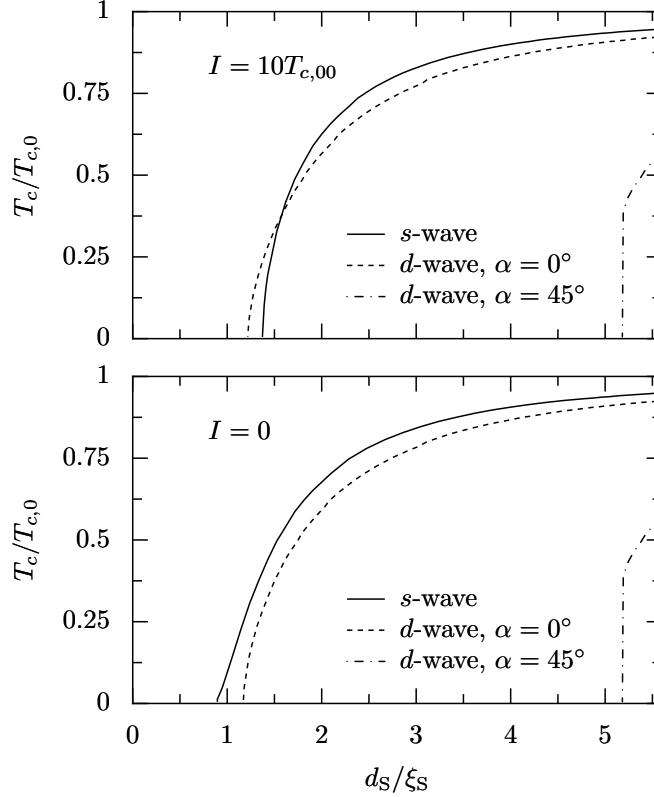


Figure 3. The critical temperature of a thin superconducting layer on top of a bulk ferromagnet ($I = 10T_{c,0}$, $d_F \rightarrow \infty$) as a function of the layer thickness, d_S , which is normalised by the superconducting coherence length ξ_S (upper panel). For comparison the critical temperature is also shown for $I = 0$ (lower panel).

oscillatory behaviour has also been observed experimentally [14, 15]. A discussion of the non-magnetic case can be found in [24].

In the following we focus on the critical temperature of bi-layer systems. As before we assume a completely transparent interface between the ferromagnet and the superconductor; furthermore the Fermi surfaces are supposed to be identical in both materials. The ferromagnet is described by the exchange energy, I , and the impurity scattering strength, $1/2\tau_F$; we choose these parameters to be $I = 10T_{c,0}$ and $1/2\tau_F = 5T_{c,0}$. This is a reasonable choice having in mind ferromagnetic metals like Fe or Ni which are well-described by the relations $T_c \ll I$, and $1/2\tau_F \ll I$.

First we study the critical temperature of the system with an s -wave superconductor, which we assume to be dirty, $1/2\tau_S = 10T_{c,0}$. The coherence length at zero temperature, ξ_S , is given by $\xi_S = \sqrt{\xi_0 l_S} \approx 0.53\xi_0$ where $\xi_0 = v_F/\Delta_0\pi$ ($\Delta_0 = 1.768T_{c,0}$) is the BCS-value of the coherence length for a clean superconductor, and $l_S = \tau_S v_F$ is the mean free path. In figure 3 we present the critical temperature, T_c , for a superconducting layer on a bulk ferromagnet ($d_F \rightarrow \infty$) as a function of its thickness, d_S . The critical temperature decreases with the thickness of the superconductor, and below a critical layer thickness, $d_S = 1.37\xi_S$, the superconductivity vanishes. Now

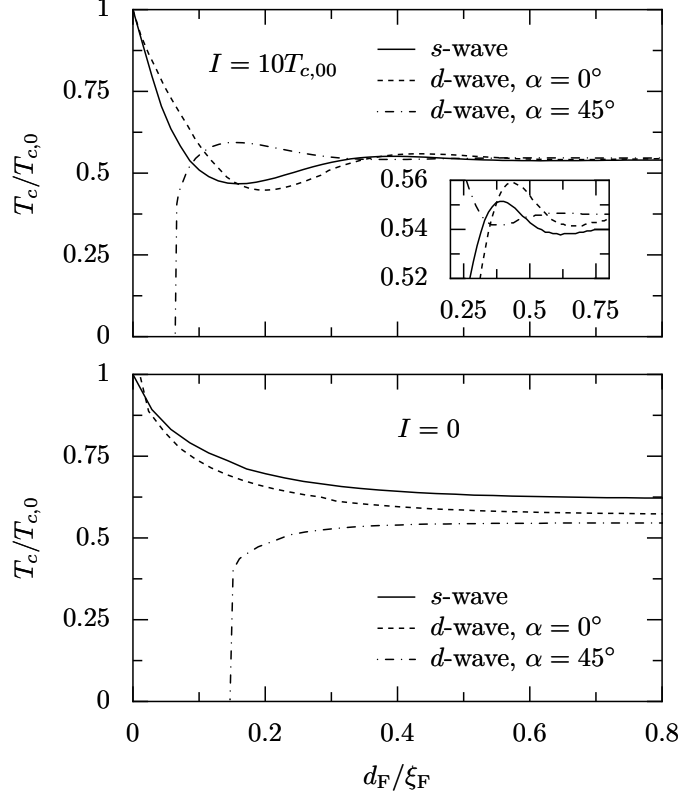


Figure 4. The critical temperature of a bi-layer with fixed d_S as a function of the ferromagnetic layer thickness d_F (upper panel). For all order parameter types T_c is oscillating. The parameter d_S is chosen such that $T_c = 0.54T_{c,0}$ for $d_F \rightarrow \infty$; i.e. d_S equals $1.72\xi_S$, $1.22\xi_S$, and $5.52\xi_S$ for the s -wave, unrotated and rotated d -wave situations, respectively. For comparison the critical temperature is also shown for the unrotated case, $I = 0$, where no oscillations occur (lower panel).

we fix $d_S = 1.72\xi_S$, for which $T_c = 0.54T_{c,0}$ when $d_F \rightarrow \infty$; for this thickness of the superconducting layer we examine the critical temperature as a function of the ferromagnetic layer thickness, d_F . We find an oscillation of the critical temperature when varying the thickness of the ferromagnet (see figure 4).

The oscillations can be explained as follows: since no current can flow across the surface at $x = d_F$, the pairing function has to obey particular boundary conditions, i.e. its derivative normal to the surface has to vanish. In the presence of a spin exchange field the pairing is spatially oscillating with wave length $\xi_F = \pi v_F/I$ [7]. At the maxima of T_c the thickness of the ferromagnetic layer, d_F , is such that the boundary conditions are fulfilled quite naturally, whereas minima occur if the pairing function has to be suppressed considerably to fulfil the boundary conditions. Therefore the distance of two neighbouring minima is expected to be of the order of $0.5\xi_F$, which is the same periodicity as observed before for the density of states (see figure 2). In our numerical calculation the first two minima of T_c can be found at $d_F = 0.16\xi_F$ and $d_F = 0.62\xi_F$ (s -wave case, see inset in figure 4). Their distance is $0.46\xi_F$ which is close to the expected value. These results are consistent with other theoretical findings [6, 7]

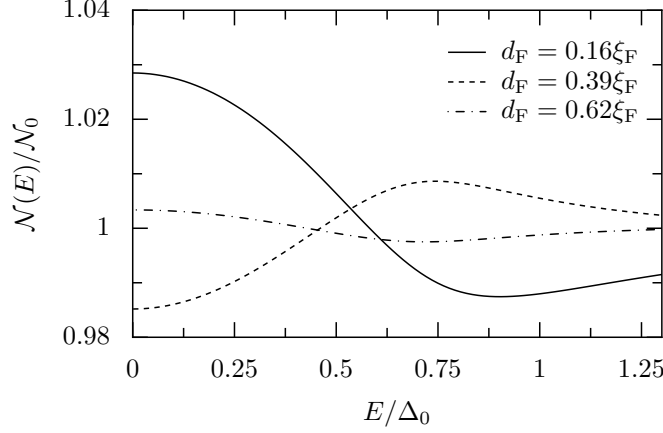


Figure 5. The density of states at $x = d_F$ for an s -wave symmetry of the order parameter. These values of d_F correspond to the first two minima ($d_F = 0.16\xi_F, 0.62\xi_F$) and the first maximum ($d_F = 0.39\xi_F$) of the critical temperature.

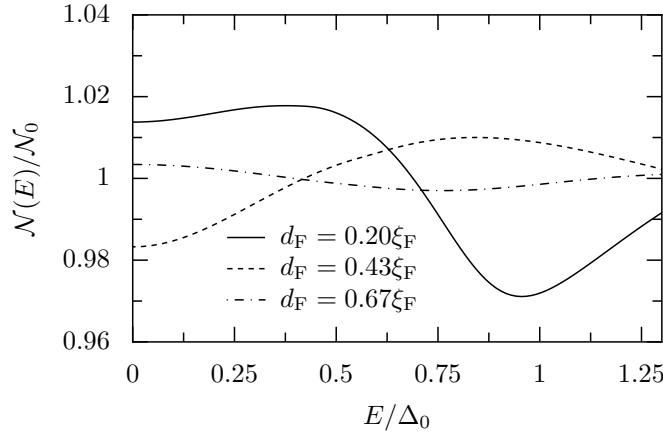


Figure 6. The density of states at $x = d_F$ for an unrotated d -wave symmetry of the order parameter. These values of d_F correspond to the first two minima ($d_F = 0.20, 0.67\xi_F$) and the first maximum ($d_F = 0.43\xi_F$) of the critical temperature.

which could also be fitted to experimental observations [3, 5]. For comparison we also present the critical temperature for a non-magnetic metal layer ($I = 0$); as expected superconductivity is suppressed less effectively without magnetism (see figure 3). For this case, no oscillations with the metal layer thickness are observed (see figure 4), which is an obvious result considering the discussion in relation with (8)-(11).

As previously discussed, the oscillating behaviour of the pairing function can also be observed in the local density of states at $x = d_F$. We calculate the density of states for those values of d_F where the critical temperature has a maximum or a minimum. The results are presented in figure 5. For the minima of T_c (at $d_F = 0.16, 0.62\xi_F$)

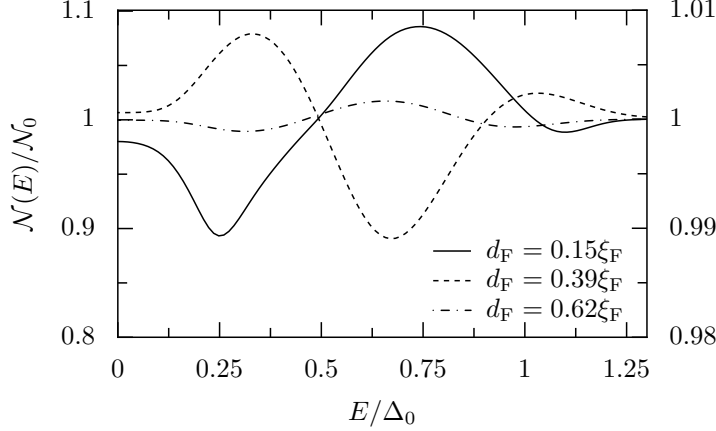


Figure 7. The density of states at $x = d_F$ for a 45° -rotated d -wave symmetry of the order parameter. The left axis applies to the density of states at the first maximum of T_c ($d_F = 0.15\xi_F$), whereas the right axis applies for the first minimum ($d_F = 0.39\xi_F$) and the second maximum ($d_F = 0.62\xi_F$).

the density of states in the gap region is enhanced compared to the normal state; this is related to sub-gap Andreev bound states which exist inside the ferromagnet. At the maximum of T_c ($d_F = 0.39\xi_F$) we find a gap-like structure of the density of states; i.e. in the gap region the density of states is smaller than the normal state value. Altogether we find that bound states in the gap region tend to suppress superconductivity, and can be related to minima of T_c .

Now we will turn to the case of d -wave superconductors. For a d -wave symmetry of the order parameter the bulk value of the critical temperature, $T_{c,0}$, is suppressed by non-magnetic impurities, and T_c is given by [25]

$$\ln\left(\frac{T_{c,00}}{T_{c,0}}\right) = \Psi\left(\frac{1}{2} + \frac{1}{4\pi T_{c,0}\tau_S}\right) - \Psi\left(\frac{1}{2}\right) \quad (13)$$

where $T_{c,00}$ is the critical temperature for a clean sample and $\Psi(x)$ is the digamma function. In the following we choose the impurity scattering inside the superconductor to be $1/2\tau_S = 0.1T_{c,00}$ which leads to $T_{c,0} = 0.92T_{c,00}$; the bulk order parameter at zero temperature is $\Delta_0 = 2.02T_{c,00}$ which is smaller than its value in the clean case ($\Delta_{00} = 2.14T_{c,00}$). As the disorder is small the superconducting coherence length is given by $\xi_S \approx \xi_0 = v_F/\Delta_0\pi$.

It is well-known that the behaviour of d -wave superconductors at boundaries depends crucially on the orientation of the order parameter with respect to the boundary. Therefore we compare the case where the order parameter is rotated by 45° with the unrotated case.

An unrotated d -wave superconductor is expected to behave similar to an s -wave superconductor. The reason is that along the classical trajectories the order parameter does not change its phase. And indeed the behaviour of an unrotated d -wave superconductor and an s -wave superconductor is quite similar: the superconductivity of a thin layer on a bulk ferromagnet is suppressed completely when its thickness is below $d_S = 1.22\xi_S$ (see figure 3). If we fix the superconducting layer thickness to $d_S = 1.94\xi_S$ (which leads to $T_c = 0.54T_{c,0}$ for $d_F \rightarrow \infty$) and vary d_F we find an

oscillating behaviour of T_c as before. The first two minima are at $d_F = 0.20\xi_F$ and $d_F = 0.67\xi_F$, and the first maximum can be found at $d_F = 0.43\xi_F$ (see figure 4); the distance between the first two minima is $0.47\xi_F$. Of course some quantitative differences exist which are mainly due to the nodes of the d -wave order parameter. The critical temperature for a non-magnetic metal layer ($I = 0$) behaves similar to the s -wave case: for an infinite metal layer T_c lies above the value for the magnetic case (see figure 3); the oscillations with a varying thickness of the non-magnetic metal vanish (see figure 4).

For those values of d_F which are related to a maximum or a minimum of T_c the density of states shows qualitatively the same behaviour as for the s -wave case; i.e. for small energies the density of states at minima of T_c is enhanced compared to the normal state value whereas a gap-like structure can be observed at the maxima of T_c (see figure 6).

The situation changes drastically if the d -wave order parameter is rotated by 45° : Surfaces are now pair-breaking as the quasi-particles are scattered so that a sign change of the order parameter occurs along their trajectories [22]; and it is well-known that at specular surfaces the order parameter vanishes. As a consequence the suppression of superconductivity is much stronger than for the cases discussed before. For a superconducting layer which is on top of a bulk ferromagnet this can be seen in figure 3; in particular the critical thickness of the superconductor, below which superconductivity vanishes, is $d_S = 5.18\xi_S$, which is much larger than in the previous situations. We now fix the layer thickness of the superconductor to $d_S = 5.52\xi_S$ so that $T_c = 0.54T_{c,0}$ for $d_F \rightarrow \infty$. When analysing T_c as a function of d_F we find a completely different behaviour than before: for $d_F = 0$ the order parameter at the pair-breaking (specular) surfaces, $x = -d_S$ and $x = 0$, must be zero. This suppression of superconductivity leads to a vanishing critical temperature of the bi-layer for $d_F < 0.06\xi_F$. The pair-breaking at $x = 0$ is weakened when the ferromagnetic layer thickness increases, and for $d_F > 0.06\xi_F$ the critical temperature becomes finite. When further increasing d_F the critical temperature is oscillating as in the previous cases, but now starting with a maximum at $d_F = 0.15\xi_F$; the first minimum can be found at $d_F = 0.39\xi_F$, and the second maximum at $d_F = 0.62\xi_F$. The difference between the first two maxima is $0.47\xi_F$ as for the unrotated order parameter. It is not surprising that the periodicity is not affected by the rotation of the order parameter because the oscillation of the pairing function is an exclusive result of the ferromagnetic exchange energy I , and is independent of details inside the superconductor. For an infinite non-magnetic metal layer ($I = 0$) the critical temperature of the rotated d -wave superconductor remains unchanged (see figure 3), as the suppression of superconductivity is not dominated by the metal layer but by the surface of the superconductor at $x = -d_S$ as discussed above. The critical temperature shows no oscillations with the thickness of the non-magnetic layer (see figure 4).

The density of states at $x = d_F$ shows a clearly different behaviour. In particular for $d_F = 0$ zero-energy Andreev bound states exist at the surfaces due to the sign change of the order parameter for scattered quasi-particles. For the first maximum of T_c ($d_F = 0.15\xi_F$) the density of states is suppressed below the normal state value (see figure 7) but a remainder of the zero-energy bound state is still observable. For the first minimum of T_c ($d_F = 0.39\xi_F$) the density of states for small energies ($E \approx 0$) is enhanced compared to the normal state value, and for the second maximum of T_c ($d_F = 0.62\xi_F$) it is suppressed, which, however, can hardly be seen in figure 7. It is remarkable that the density of states in the gap region has more structure here than in

the previous case. This is due to the strong angular dependence of the order parameter close to those directions which are perpendicular to the interface. Altogether, for an 45° -rotated d -wave order parameter, we also find that the minima of T_c are related to an enhanced density of states in the sub-gap region, and vice versa for the maxima of T_c .

4. Conclusion

We have studied superconductor-ferromagnet bi-layers for s -wave and d -wave superconductors. In all discussed cases we observed an oscillating behaviour of the density of states as well as of the critical temperature when varying the thickness of the ferromagnetic layer. The origin of these oscillations is the exchange field in the ferromagnetic metal which leads to a Larkin-Ovchinnikov-Fulde-Ferrell-like state with a spatially oscillating pairing function. In particular we find that the density of states in the ferromagnetic layer is enhanced in the gap region when its thickness leads to a minimum of the critical temperature. When the critical temperature has a maximum the density of states in the ferromagnetic layer has a gap-like structure.

Comparing the different order parameter symmetries, we observe a similar behaviour for the s -wave and the unrotated d -wave cases. The critical temperature as a function of the ferromagnetic layer thickness, d_F , decreases for small values of d_F ($d_F < 0.2\xi_F$) and shows oscillations around an asymptotic value of T_c when further increasing d_F . In the s -wave case these findings are in agreement with previous theoretical studies [6, 7], and are also experimentally confirmed [3, 4, 5].

This behaviour is considerably modified if the d -wave superconductor is rotated by 45° with respect to the surface. In this case superconductivity may even vanish for very thin ferromagnetic layers. If d_F exceeds a critical value, superconductivity can be restored and oscillations around the asymptotic value of T_c are observed. This difference in behaviour is due to the sign change of the order parameter for quasi-particles which are scattered at the surface, which leads to a suppression of superconductivity. It would be most interesting to check our results for d -wave superconductors also experimentally.

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